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GLOBAL SENSITIVITY ANALYSIS FOR STOCHASTIC PROCESSES WITH INDEPENDENT INCREMENTS

EMELINE GAYRARD, CÉDRIC CHAUVIÈRE, HACÈNE DJELLOUT, PIERRE BONNET, AND DON-PIERRE ZAPPA

ABSTRACT. This paper is a first attempt to develop a numerical technique to analyze the sensitivity and the propagation of uncertainty through a system with stochastic processes having independent increments as input. Similar to Sobol' indices for random variables, a metamodel based on Chaos expansions is used and it is shown to be well suited to address such problems. New global sensitivity indices are also introduced to tackle the specificity of stochastic processes. The accuracy and the efficiency of the proposed method is demonstrated on an analytical example with three different input stochastic processes: a Wiener process; an Ornstein-Uhlenbeck process and a Brownian bridge process. The considered output, which is function of these three processes, is a non-Gaussian process. Then, we apply the same ideas on an example without known analytical solution.

Key words: Stochastic processes, Sobol' indices, Chaos expansions, Orthogonal polynomial.

AMS 2010 subject classifications. 90B22, 60K25, 65C05, 65C50

1. Introduction

Many engineering problems have input parameters that are not precisely known. They are usually modeled as random variable and the propagation of uncertainty through the system may be treated in several ways, going from rough Monte Carlo simulations [8], interval arithmetic [16] or Taylor series expansion [17], to quote a few. The interested reader may also refer to the overviews [10, 12, 29], for example.

On the other hand, sensitivity analysis aims at identifying the input parameters whose uncertainty has the largest impact on the variability of some output quantities. They are two major categories: local sensitivity analysis and global sensitivity analysis. The first one is usually based on the gradient or the partial derivatives of output quantities and studies the variability in the vicinity of some set of points. One may refer to the paper of Zhou et al. [32] for a detailed overview of techniques belonging to that category. In this paper, we are concerned with the global sensitivity analysis of systems involving random processes, and more specifically indices belonging to Sobol's family. Those are variance-based indices and have received much attention from the mathematical and the engineering community over the past twenty years or so [1, 21, 26].

Polynomial Chaos as a meta-model has been popularized by Ghanem and Spanos [6] in the 90's and later generalized by Xiu and Karniadakis [30, 31].

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Since the seminal work of Sudret [24], it quickly became obvious that using Polynomial Chaos expansion as meta-model was one of the most straightforward and efficient way of computing Sobol' indices.

Ever since, the work of researchers has spread in many directions. One of them, consists in building meta-model more efficiently, using sparse Polynomial Chaos expansion, for example [4]. Others have tried to adapt Sobol' indices for dependent input random variables, leading to different family of global sensitivity indices [2, 9, 13, 15]. Those have been compared with other global indices (Shapely and f-sensitivity, in particular); see [18, 19, 22], for example.

In this paper, we tackle the problem of defining Sobol' indices for input stochastic processes with independent increments. Assuming a model of the form $Y_t = g(X_t^1, ..., X_t^d)$, with $(X_t^1, ..., X_t^d)$ d independent input stochastic processes, we explain why the output considered should be $Y_t - Y_s$ instead of just Y_t . Then, our sensitivity analysis on $Y_t - Y_s$ can be recasted into the standard formalism of independent random variables by considering stochastic processes with independent increments. To the best of our knowledge, this paper is a first attempt to adapt Sobol' indices with stochastic processes as input variables. The reason why such problem has long been a challenge for researchers lies in the high dimensionality of stochastic processes. All current techniques trip on the so-called curse of dimensionality. In this paper, we rely on the independence of the increments of stochastic processes to handle the curse of dimensionality.

In order to make the paper self-contained, some materials that can be considered as classical and that may be found in different other places are restated. This is why the next section is devoted to recall some important notions about orthogonal polynomial and Chaos expansion [25, 28]. Then, the computation of Sobol' indices from the coefficients of Chaos polynomials is given in the context of random variables. We then move on to adapt the same ideas for input random processes with independent increments. Section 4 applies the proposed approach to two numerical examples: one with an analytical solution and one without analytical solution. The last section provides some possible extensions and concluding remarks.

2. Polynomial Chaos Expansion

Polynomial Chaos expansion has long been an efficient way of building a meta model from which macroscopic quantities may be computed efficiently. The next two subsections restate some of its main features.

2.1. Orthogonal Polynomials.

The most popular way to build such polynomials relies on the three-term recurrence relation (see Gautschi [5] for more details). Let V^d denotes the real vector space of all polynomials in d variables with real coefficients, together with the positive inner product on V^d defined as

$$\langle u, v \rangle = \int_{I} u(\mathbf{x})v(\mathbf{x})f(\mathbf{x})d\mathbf{x} \ \forall u, v \in V^{d},$$
 (1)

where $f:I\subset\mathbb{R}^d\to\mathbb{R}^+$ is a positive integrable function of $\mathbf{x}=(x_1,x_2,\ldots,x_d)$. We also assume that the weight function f can be written as the product of univariate weight functions, i.e. $f(x_1,x_2,...,x_d)=f_1(x_1)f_2(x_2)\ldots f_d(x_d)$, where $f_i:I_i\subset\mathbb{R}\to\mathbb{R}^+$ are positive integrable functions. Then, the multivariate polynomial basis of degree d with (P_d^p+1) elements $\{\Psi_0(\mathbf{x}),\Psi_1(\mathbf{x}),...,\Psi_{P_d^p}(\mathbf{x})\}$ is built from the tensor product of the elements of a univariate polynomial basis, of degree n i.e.

$$\Psi_{\alpha_1...\alpha_d}(\mathbf{x}) = \prod_{i=1}^d \Psi_{\alpha_i}(x_i), \tag{2}$$

where $\alpha_i \in \{0, 1, ..., n\}$. Nevertheless, not all the elements of the form (2) are kept when constructing the multivariate polynomial basis (that would lead to an incomplete basis of degree nd with $(n+1)^d$ elements). Instead, for

a given degree p, only the elements that satisfy $\sum_{i=0}^{d} \alpha_i \leq p$ in (2) are retained

and a one to one correspondence between the multi-index $(\alpha_0, \ldots, \alpha_d)$ and the i^{th} element $\Psi_i(\mathbf{x})$ of the multivariate basis is established. Doing so, it can be shown that the number of elements of a multivariate polynomial basis of degree p is

$$P_d^p + 1 = \binom{p+d}{d} = \frac{(p+d)!}{d! \ p!}.$$
 (3)

Then, any function $u: I \subset \mathbb{R}^d \to \mathbb{R}$ sufficiently regular may be approximated by its projection $\Pi_p u$ on such basis, i.e.

$$\Pi_p u(\mathbf{x}) = \sum_{i=0}^{P_d^p} \widehat{u}_i \Psi_i(\mathbf{x}), \tag{4}$$

where \hat{u}_i are the coordinates of the projection of u onto the basis $\{\Psi_i\}_{0 \leq i \leq P_d^p}$. The ideas presented above in a deterministic context may also be efficiently used in the field of probability, where orthogonal polynomials are usually referred to as Polynomial Chaos (PC).

2.2. Polynomial Chaos expansion.

We now denote by $(\Omega, \mathcal{A}, \mathbb{P})$ the probability space, where Ω is the set of all possible outcomes, \mathcal{A} is a σ -algebra over Ω , and \mathbb{P} is a function $\mathcal{A} \to [0, 1]$ that gives a probability measure on \mathcal{A} . Let $I = I_1 \times ... \times I_d$ be a domain of \mathbb{R}^d and $\mathbf{X} = (X_1, \dots, X_d)$ be an I-valued independent random vector that describes input uncertainties. The probability law of \mathbf{X} can be defined by the probability density function

$$f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^{d} f_i(x_i), \tag{5}$$

where $f_i: I_i \to \mathbb{R}^+$ is the marginal probability density of X_i defined on $(\Omega_i, \mathcal{A}_i, \mathbb{P}_i)$. Let $L_2(\Omega_i, \mathcal{A}_i, \mathbb{P}_i)$ denotes the space of real random variables with finite second order moments, i.e. such that

$$\mathbb{E}(X_i^2) = \int_{I_i} x_i^2 f_i(x_i) dx_i < \infty, \tag{6}$$

where \mathbb{E} is the mathematical expectation. The Hilbert spaces $L_2(\Omega_i, \mathcal{A}_i, \mathbb{P}_i)$ can be provided with a set of complete orthogonal basis $\{\Psi_j^i(x)\}_{j\geq 0}$ that are consistent with the density of X_i . For example, Hermite polynomials are associated with Gaussian distributions and Legendre polynomials are associated with uniform distributions. In the same manner, $L_2(\Omega, \mathcal{A}, \mathbb{P})$ is provided with a set of complete multivariate orthogonal basis $\{\Psi_j(\mathbf{x})\}_{j\geq 0}$ which, in turn, is consistent with the density of \mathbf{X} .

Let $Y = Y(X_1, ..., X_d) : \Omega \to \mathbb{R}$ represent a mathematical model belonging to $L_2(\Omega, \mathcal{A}, \mathcal{P})$. Then, it can be represented as [6, 30]

$$Y(X_{1},..,X_{d}) = z_{0}\Psi_{0} + \sum_{i_{1}=1}^{\infty} z_{i_{1}}\Psi_{1}(X_{i_{1}}) + \sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} z_{i_{1}i_{2}}\Psi_{2}(X_{i_{1}},X_{i_{2}}) + \sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \sum_{i_{2}=1}^{i_{2}} z_{i_{1}i_{2}i_{3}}\Psi_{3}(X_{i_{1}},X_{i_{2}},X_{i_{3}}) + \cdots,$$

$$(7)$$

which, after some rearranging, can be rewritten in a more convenient way as

$$Y(\mathbf{X}) = \sum_{j=0}^{\infty} y_j \Psi_j(\mathbf{X}). \tag{8}$$

Similarly to equation (4), the above series is truncated by keeping terms up to a degree p

$$Y(\mathbf{X}) \approx \Pi_p Y(\mathbf{X}) = \sum_{j=0}^{P_d^p} y_j \Psi_j(\mathbf{X}). \tag{9}$$

The way to compute the PC coefficients $\{y_j\}_{0 \leq j \leq P_d^p}$ of equation (9) can be split into two different families: projection methods and regression methods [20]. Here, we use the first one which consists in premultiplying (9) by $\Psi_j(\mathbf{X})$ and by taking the expectation of the resulting product. The orthogonality of the PC basis cancels most of the terms, leading to

$$y_j = \mathbb{E}(Y(\mathbf{X})\Psi_j(\mathbf{X})) = \int_I Y(\mathbf{x})\Psi_j(\mathbf{x})f_{\mathbf{X}}(\mathbf{x})d\mathbf{x} \text{ for } j = 0, 1..., P_d^p.$$
(10)

2.3. Computing PC coefficients.

The method to evaluate the integral (10) is mainly determined by the dimension d of the input random. For high values of d, Monte-Carlo sampling simulation is the method of choice. For moderate values of d, Gaussian quadrature rules remain most effective and between those two extreme cases, sparse quadrature rules might be a good choice. In this paper, the maximum value of d is d=6, so we evaluate such integrals using Gaussian quadrature rules [7] of the form

$$\int_{I} Y(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \approx \sum_{i_1=1}^{N_{g_1}} \sum_{i_2=1}^{N_{g_2}} \dots \sum_{i_d=1}^{N_{g_d}} \omega_{i_1} \omega_{i_2} \dots \omega_{i_d} Y(\widetilde{x}_{i_1}, \widetilde{x}_{i_2} \dots, \widetilde{x}_{i_d}), \tag{11}$$

where $\{\omega_{i_k}\}_{1\leq i_k\leq N_{g_k}}$ are the quadrature weight and $\{\widetilde{x}_{i_k}\}_{1\leq i_k\leq N_{g_k}}$ are the quadrature points. The Gaussian quadrature rules are built such that the integral is exact if Y is a multivariate polynomial containing monomials x_{i_k}

of maximum degree $2N_{g_k}-1$. From equations (10) and (11), we see that it necessary to evaluate the response Y at $N_{g_1} \times N_{g_2} \dots \times N_{g_d}$ deterministic quadrature points $(\widetilde{x}_{i_1}, \widetilde{x}_{i_2}, \widetilde{x}_{i_d})$ in order to compute the PC coefficients. Since $\Psi_0 = 1$, it can easily be shown that the first coefficient of the PC expansion is the expectation of the random response of the system, i.e.

$$\mathbb{E}(Y(\mathbf{X})) = y_0. \tag{12}$$

Similarly, by considering the approximation of Y^2

$$Y(\mathbf{X})^2 \approx \sum_{i=0}^{P_d^p} \sum_{j=0}^{P_d^p} y_i y_j \Psi_i(\mathbf{X}) \Psi_j(\mathbf{X}), \tag{13}$$

and taking the expectation on each side, the orthogonality of the PC basis leads to

$$\mathbb{E}(Y(\mathbf{X})^2) = \sum_{i=0}^{P_d^p} y_i^2,\tag{14}$$

from which the variance of the random response of the system can be evaluated. The PC decomposition not only provides a convenient way to compute first and second order moments, but also Sobol' indices, as will be explained in the next section.

3. Sensitivity Analysis

3.1. Sobol' indices for random variables.

As in the previous section, we consider the mathematical model $Y = Y(\mathbf{X})$ and we assume that Y belong to $L_2(\Omega, \mathcal{A}, \mathbb{P})$. Sobol has shown that any square integrable function could be expressed as the sum of 2^d terms of increasing dimension such that

$$Y(\mathbf{x}) = Y_0 + \sum_{i_1=1}^d Y_{i_1}(x_{i_1}) + \sum_{1 \le i_1 < i_2 \le d} Y_{i_1 i_2}(x_{i_1}, x_{i_2}) + \dots + Y_{i_1 \dots i_d}(x_{i_1}, \dots, x_{i_d}),$$
(15)

with

$$\int_{I_{i_k}} Y_{i_1...i_s}(x_{i_1},..,x_{i_s}) dx_{i_k} = 0 \text{ for } k \in \{1,...,s\} \text{ and } s \in \{1,...,d\}.$$
 (16)

The above property ensures the uniqueness of the decomposition together with the pairwise orthogonality of the functions appearing into equation (15), with respect to the dot product defined by equation (1). Thus, the total variance of Y denoted by V(Y) can be decomposed as follows:

$$V(Y) = \sum_{i_1=1}^{d} V(Y_{i_1}(X_{i_1})) + \sum_{1 \le i_1 < i_2 \le d} V(Y_{i_1 i_2}(X_{i_1}, X_{i_2})) + \cdots + V(Y_{i_1 ... i_d}(X_{i_1}, ..., X_{i_d}))$$

$$= \sum_{i_1=1}^{d} V_{i_1} + \sum_{1 \le i_1 < i_2 \le d} V_{i_1 i_2} + \cdots + V_{i_1 ... i_d},$$

$$(17)$$

where

$$V_{i_{1}} = V(\mathbb{E}(Y/X_{i_{1}}))$$

$$V_{i_{1}i_{2}} = V(\mathbb{E}(Y/X_{i_{1}}, X_{i_{2}})) - V_{i_{1}} - V_{i_{2}}$$

$$V_{i_{1}i_{2}i_{3}} = V(\mathbb{E}(Y/X_{i_{1}}, X_{i_{2}}, X_{i_{3}})) - V_{i_{1}i_{2}} - V_{i_{1}i_{3}} - V_{i_{2}i_{3}} - V_{i_{1}} - V_{i_{2}} - V_{i_{3}}$$

$$\cdots$$

$$(18)$$

$$V_{i_1...i_d} = V - \sum_{i=1}^d V_i - \sum_{1 \le i_1 < i_2 \le d} V_{i_1 i_2} - \dots - \sum_{1 \le i_1 < i_2 ... < i_{d-1} \le d} V_{i_1...i_{d-1}}$$

Then, Sobol' indices of order k introduced in 1993 in [23] are given by

$$S_{i_1\dots i_k} = \frac{V_{i_1\dots i_k}}{V}. (19)$$

In particular, the first order Sobol' indices that measures the influence of the input parameter X_i is defined by

$$S_i = \frac{V(\mathbb{E}(Y/X_i))}{V(Y)} = \frac{V_i}{V}.$$
 (20)

Although Sobol' indices could be computed by estimating integrals appearing into equations (18), that would be both computationally expensive and hardly tractable. In the seminal work of Sudret [24], it is noticed that PC expansion has exactly the same structure and property as Sobol' decomposition (15). This is why such meta model has met such a tremendous success when it comes to computing Sobol' indices. Let denote by $I_{i_1,i_2,...,i_s}$ ($s \leq d$) the set of d-dimensional vectors $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d)$ with $\boldsymbol{\alpha} \neq \boldsymbol{0}$ and $0 \leq \alpha_1 \leq \ldots \leq \alpha_d \leq d$ that selects elements of the PC basis $\Psi_{\alpha_1...\alpha_d}$ defined by (2) containing solely the variables $X_{i_1}, X_{i_2}, \ldots, X_{i_s}$. For example, the multi-indices defined by I_i will select elements of the PC basis depending only on the variable X_i . Similarly, $I_{i,j}$ will select elements of the PC basis that depend on X_i and X_j , to the exclusion of any other variable. With this notation, Sobol's indices of order k are simply given as a function of the PC coefficients as follows (see [24] for details):

$$S_{i_1...i_k} = \frac{1}{V} \sum_{(\alpha_1,...,\alpha_d) \in I_{i_1,...,i_k}} y_{\alpha_1...\alpha_d}^2.$$
 (21)

For a problem with d input random parameters, (2^d-1) Sobol' indices can be computed and when d is large, it becomes difficult to draw conclusions from these too numerous indices. This is why, in 1996, Homma and Saltelli [11] introduced the total sensitivity indices S_{T_i} ($i=1,\ldots,d$) which measures the total effect of the i^{th} random input parameter. It is defined as the sum of all sensitivity indices $S_{i_1...i_k}$ ($k=1,\ldots,d$) for which, one of the indices i_1,i_2,\ldots,i_k is equal to i, i.e.

$$S_{T_i} = \sum_{\substack{k=1\\(i_1,\dots,i_k)\in J_i^k}}^d S_{i_1\dots i_k},\tag{22}$$

where J_i^k is the set of k-dimensional vectors (i_1, \ldots, i_k) with $1 \le i_1 < \ldots < i_k \le d$, such that one of its components is equal to i. These indices can also

be computed from the PC expansion as follows:

$$S_{T_i} = 1 - \frac{1}{V} \sum_{(\alpha_1, \dots, \alpha_d) \in \overline{I}_i} y_{\alpha_1 \dots \alpha_d}^2, \tag{23}$$

where \overline{I}_i is the complementary set of I_i .

3.2. Sobol' indices for processes with independent increments.

Let $(X_t^i)_{t\in[0;T_f]}^{i\in\{1,\dots d\}}$ denote d independent stochastic processes with independent increments on a filtered probability space $(\Omega, \mathcal{A}, (\mathcal{A}_t)_{t\in[0;T_f]}, \mathbb{P})$. For notation convenience we gather those processes into a vector $\mathbf{X}_t = (X_t^1, \dots, X_t^d)$ and we assume that a physical model is represented by a function $g: \mathbb{R}^d \to \mathbb{R}$ such that $Y_t = g(\mathbf{X}_t)$. Since X_t^1, \dots, X_t^d are independent processes, for a fixed value of t, they can be seen as independent random variables and Sobol' indices described in the previous sections could be straightforwardly used. However, doing so, a key property of stochastic processes is not taken into account. Indeed, for $(s,t) \in [0,T_f] \times [0,T_f]$, with s < t, \mathbf{X}_t and \mathbf{X}_s are dependent and this should be reflected in the model output. This is why instead of considering Y_t for the model output, it is essential to consider $Y_t - Y_s$ for all $(s,t) \in [0,T_f]^2$ and perform a sensitivity analysis on that quantity. Thus, in this section, we introduce Sobol' indices for the model

$$Y_t - Y_s = g(\mathbf{X}_t) - g(\mathbf{X}_s)$$

$$= G(\mathbf{X}_t, \mathbf{X}_s),$$
(24)

where the function $G: \mathbb{R}^{2d} \to \mathbb{R}$ is such that its arguments \mathbf{X}_t and \mathbf{X}_s are now dependent. The essential point in the proposed procedure is to transform the G function into a function whose arguments will be independent. This is why we choose processes with independent increments at the entry.

Let's introduce the following notation (for $(s,t) \in [0,T_f]^2$ and $i \in \{1,...d\}$):

$$\Delta_s^t X^i = X_t^i - X_s^i \tag{25}$$

with $X_0^i = 0$. Then, for $i \in \{1, ...d\}$, $\Delta_s^t X^i$ is independent from $\Delta_{s'}^{t'} X^i$ for all s, t, s', t' such as $0 < s < t \le s' < t'$. We introduce the vector $\Delta_s^t \mathbf{X} = (\Delta_s^t X^1, ..., \Delta_s^t X^d)$ such that, we can write

$$Y_t - Y_s = G(\mathbf{X}_t, \mathbf{X}_s)$$

$$= G(\Delta_s^t \mathbf{X} + \mathbf{X}_s, \mathbf{X}_s)$$

$$= G(\Delta_s^t \mathbf{X} + \Delta_0^s \mathbf{X}, \Delta_0^s \mathbf{X})$$

$$= H(\Delta_s^t \mathbf{X}, \Delta_0^s \mathbf{X})$$
(26)

with the function $H: \mathbb{R}^{2d} \to \mathbb{R}$ such that its arguments $\Delta_s^t \mathbf{X}$ and $\Delta_0^s \mathbf{X}$ are now independent. For fixed values of s and t into $[0, T_f]$, we define the random variables N_i $(i \in \{1, ... 2d\})$ by

$$N_{i} = \begin{cases} \Delta_{s}^{t} X^{i} & \text{for } i = 1, ..., d \\ \Delta_{0}^{s} X^{i-d} & \text{for } i = d+1, ..., 2d \end{cases},$$
 (27)

and we gather those independent random variables into a 2d dimensional vector $\mathbf{N} = (N_1, ..., N_{2d})$ so that our model now writes

$$Y_t - Y_s = H(\mathbf{N}). \tag{28}$$

Q

By proceeding that way, we have transformed our initial problem with 2d dependent random processes at the entry into a problem with 2d independent random variables (for s and t fixed into $[0, T_f]$). Therefore, Sobol' indices described in the previous section can be used as is on the function $H(\mathbf{N})$, provided that this function is square integrable. It should be noted that Sobol' indices are now functions of two variables (s,t). For example, for i=1,...,d

$$S_{i}(s,t) = \frac{V(\mathbb{E}(Y_{t} - Y_{s}|N_{i}))}{V(Y_{t} - Y_{s})}$$

$$= \frac{V(\mathbb{E}(Y_{t} - Y_{s}|\Delta_{s}^{t}X^{i}))}{V(Y_{t} - Y_{s})}$$

$$= \frac{V(\mathbb{E}(Y_{t} - Y_{s}|X_{t}^{i} - X_{s}^{i}))}{V(Y_{t} - Y_{s})}.$$
(29)

Setting s=0, in the above expression leads to the standard variance decomposition with Sobol' indices of $V(Y_t)$. The interpretation of these indices is as follows: considering two points s and t of the trajectory of a process, $S_i(s,t)$ represents the influence of the i^{th} entry stochastic process $\Delta_s^t X^i$ on the same two points of the output process $\Delta_s^t Y = Y_t - Y_s$. This is illustrated in Figure 1 that shows a sample path of $(X_t^i)_{t \in [0,T_f]}$ and the corresponding sample path of $(Y_t)_{t \in [0,T_f]}$ together with the quantities $\Delta_s^t X^i$ and $\Delta_s^t Y$ on those trajectories.

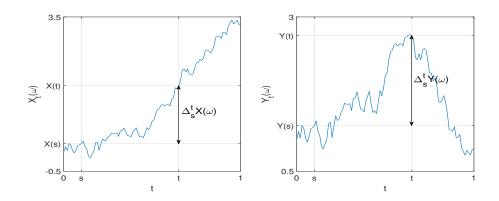


FIGURE 1. Sample path of $(X_t^i)_{t\in[0,T_f]}$ and $(Y_t)_{t\in[0,T_f]}$

Note that the last d random variables of the vector \mathbf{N} are unimportant in terms of interpretation since they have been introduced for the sole purpose of decoupling \mathbf{X}_t from \mathbf{X}_s (see equations (26)). Nevertheless, they may be useful for computing total Sobol' indices, since

$$S_{T_i}(s,t) = \sum_{\substack{k=1\\(i_1,\dots,i_k)\in J_i^k}}^{2d} S_{i_1\dots i_k}(s,t),$$
(30)

where the notations are the same as in section 3.1.

4. Examples of application

In this section, we consider two examples from which a meta-model based on Polynomial Chaos is constructed. Sobol' indices are computed from the coefficients of the PC expansion. The first one is an academic example, so that numerical results can be compared with the exact solution.

4.1. Analytical example.

Here we consider the following mathematical model for Y_t (also known as Ishigami function, [14]):

$$Y_t = g(B_t, M_t, Z_t) = a \sin^2(M_t) + (1 + bZ_t^4) \sin(B_t)$$
(31)

where a and b are some constants and (B_t) , (M_t) and (Z_t) are three independent stochastic processes defined by

$$M_t = e^t(K_t - 1) = \int_0^t e^s dL_s \qquad Z_t = \frac{O_t - 1}{T - t} = \int_0^t \frac{1}{T - u} dW_u$$
 (32)

with (B_t) , (L_t) and (W_t) three independent Brownian motions and T a positive parameter. Note that (K_t) is an Ornstein-Uhlenbeck process, (O_t) a Brownian bridge and (W_t) a Wiener process. All three are Gaussian with independent increments. By adopting the same approach as in section 3.2, we have

$$Y_{t} - Y_{s} = g(B_{t}, M_{t}, Z_{t}) - g(B_{s}, M_{s}, Z_{s})$$

$$= g((B_{t} - B_{s}) + B_{s}, (M_{t} - M_{s}) + M_{s}, (Z_{t} - Z_{s}) + Z_{s})$$

$$-g(B_{s}, M_{s}, Z_{s})$$

$$= H(B_{t} - B_{s}, M_{t} - M_{s}, Z_{t} - Z_{s}, B_{s} - B_{0}, M_{s} - M_{0}, Z_{s} - Z_{0})$$
(33)

where the function $H: \mathbb{R}^6 \to \mathbb{R}$ can be explicitly written as

$$H(x_1, x_2, x_3, x_4, x_5, x_6) = a \sin^2(x_2 + x_5) + (1 + b(x_3 + x_6)^4) \sin(x_1 + x_4) - a \sin^2(x_5) - (1 + b(x_6)^4) \sin(x_4)$$
(34)

It is this function that will be projected onto a PC basis and that will serve to compute Sobol' indices. Hermite polynomials are used to build the multivariate basis. They are orthogonal with respect to a dot product defined with a Gaussian density with zero means, and variances given below

$$\sigma_1^2 = t - s \qquad \sigma_4^2 = s
\sigma_2^2 = \frac{e^{2t} - e^{2s}}{2} \qquad \sigma_5^2 = \frac{e^{2s} - 1}{2}
\sigma_3^2 = \frac{t - s}{(T - t)(T - s)} \qquad \sigma_6^2 = \frac{s}{T(T - s)}$$
(35)

For this academic example, results can be compared with the exact value of the indices that can be computed with the following formula (valid for $t \neq s$):

$$S_{1}(s,t) = \frac{V(\mathbb{E}(Y_{t} - Y_{s}|B_{t} - B_{s}))}{V(Y_{t} - Y_{s})},$$

$$S_{2}(s,t) = \frac{V(\mathbb{E}(Y_{t} - Y_{s}|M_{t} - M_{s}))}{V(Y_{t} - Y_{s})},$$

$$S_{3}(s,t) = \frac{V(\mathbb{E}(Y_{t} - Y_{s}|Z_{t} - Z_{s}))}{V(Y_{t} - Y_{s})},$$
(36)

for the first order indices, and

$$S_{12}(s,t) = \frac{V(\mathbb{E}(Y_t - Y_s | B_t - B_s, M_t - M_s))}{V(Y_t - Y_s)} - S_1(s,t) - S_2(s,t), (37)$$

$$S_{13}(s,t) = \frac{V(\mathbb{E}(Y_t - Y_s | B_t - B_s, Z_t - Z_s))}{V(Y_t - Y_s)} - S_1(s,t) - S_3(s,t),$$

$$S_{23}(s,t) = \frac{V(\mathbb{E}(Y_t - Y_s | M_t - M_s, Z_t - Z_s))}{V(Y_t - Y_s)} - S_2(s,t) - S_3(s,t),$$

for the second order indices. The exact expression of the quantities appearing into equations (36)-(37) can be found in the appendix. For the numerical simulations, the parameters are taken equal to a = 7, b = 0.1, T = 1.1 and $(s,t) \in [0,1]^2$. The function (34) is projected onto a multivariate PC basis of degree 12.

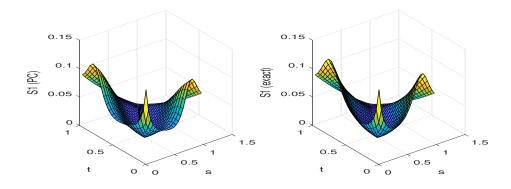


FIGURE 2. The first order index S_1 for PC expansion (left) and for the exact solution (right)

Figures 2-3 show the first order indices and Figure 4 show the second order index for both the exact solution (left) and the numerical solution (right). Only non-zeros indices are represented. We see that a degree 12 multivariate polynomial is sufficient to accurately represent our model since the exact and the approximated indices match very well. Note that it is not necessary to have a high degree of accuracy for Sobol' indices since the information to be considered is the relative importance of those indices.

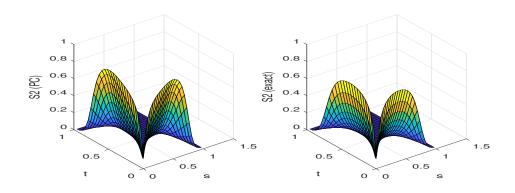


FIGURE 3. The first order index S_2 for PC expansion (left) and for the exact solution (right)

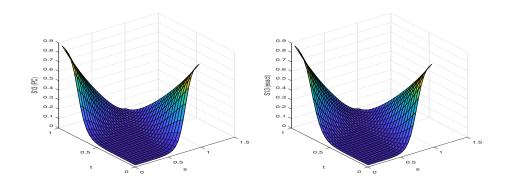


FIGURE 4. The second order index $S_{1,3}$ for PC expansion (left) and for the exact solution (right)

Multivariate polynomial degree	$E(S_1)$	$E(S_2)$	$E(S_{13})$
6			5.16×10^{-2}
12			1.35×10^{-3}
18	1.17×10^{-3}	4.51×10^{-3}	1.03×10^{-3}
24	8.19×10^{-5}	5.96×10^{-5}	2.77×10^{-4}
30	6.46×10^{-5}	1.48×10^{-5}	2.60×10^{-4}

Table 1. L^2 norm of the error of Sobol' indices S_1 , S_2 and S_{13} for increasing multivariate PC approximation degrees.

The L^2 norm of the error of a Sobol' indice S over the domain of computation is defined by

$$E(S) = \iint_{[0,1]^2} (S^a(s,t) - S^e(s,t))^2 \, \mathrm{d}s \, \mathrm{d}t,$$

where S^a and S^e stands for the approximate and the exact value of S. We compute these errors for the non-zeros indices using Fejer's quadrature rule [3]. Table 1 gives the error for increasing polynomial degrees and shows the

accuracy of the proposed method. All the univariate polynomials have the same degree in each of the six dimensions, so that the total degree of the multivariate PC expansion is a multiple of six.

In terms of interpretation, we see that the relative importance of the input $\Delta_s^t X^i$ on the output $\Delta_s^t Y$ strongly depends on the value of |s-t|. For example, S_2 and S_{13} show that for $s \simeq t$, the input stochastic processes associated with those indices have no influence on the output. On the other hand, for $s \simeq t \simeq 0$, S_1 shows that $B_t - B_s$ has a strong influence on the output.

4.2. Numerical example without analytical solution.

4.2.1. Description of the deterministic problem.

In this section, we study the deterministic trajectory of a projectile subject to air resistance modeled by a force proportional to the square of the velocity. In that case, no analytical solution exists and one has to resort to numerical techniques in order to compute the range of the projectile.

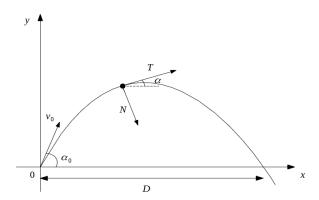


FIGURE 5. Local Frenet coordinates system and trajectory of the projectile

Assuming a drag force of the form $F_d(v) = \lambda v^2$, with λ a parameter and v the velocity of the projectile, Newton's second law of motion projected onto the local Frenet coordinates system (\mathbf{N}, \mathbf{T}) (see Figure 5) writes

$$\begin{cases}
 m\gamma_T = -mg\sin(\alpha) - \lambda v^2 \\
 m\gamma_N = mg\cos(\alpha)
\end{cases} ,$$
(38)

with m the mass of the projectile, and g the gravitational constant. The tangential and normal acceleration γ_T and γ_N can be related to the velocity through the equations $\gamma_T = \frac{dv}{dt}$ and $\gamma_N = \frac{v^2}{r}$ (the centripetal acceleration). Furthermore, we have $v = \frac{ds}{dt} = \frac{ds}{d\alpha} \frac{d\alpha}{dt} = (-r) \times \frac{d\alpha}{dt}$, by definition of the

curvature radius. Using those last equations, (38) becomes

$$\begin{cases}
 m \frac{dv}{dt} &= -mg\sin(\alpha) - \lambda v^2 \\
 \frac{v^2}{r} &= -v \frac{d\alpha}{dt} &= g\cos(\alpha)
\end{cases}$$
(39)

Following [27], we divide the two equations of (39), which leads to the following differential equation for v:

$$\frac{m\frac{dv}{dt}}{-v\frac{d\alpha}{dt}} = \frac{-mg\sin(\alpha) - \lambda v^2}{g\cos(\alpha)},$$

which gives

$$\frac{1}{v}\frac{dv}{d\alpha} = \tan(\alpha) + \frac{\lambda v^2}{mq\cos(\alpha)}.$$
 (40)

Assuming the initial condition $v(\alpha_0) = v_0$ for the velocity (see Figure 5) the solution to the differential equation (40) writes

$$v^{2}(\alpha) = \frac{v_{0}^{2}\cos^{2}(\alpha_{0})}{\cos^{2}(\alpha)\left(1 - \frac{v_{0}^{2}}{v_{lim}^{2}}\cos^{2}(\alpha_{0})\left[\ln(\tan(\frac{u}{2} + \frac{\pi}{4})) + \frac{\sin(u)}{\cos^{2}(u)}\right]_{\alpha_{0}}^{\alpha}\right)}, (41)$$

with the limit velocity v_{lim} defined by

$$v_{lim} = \sqrt{\frac{mg}{\lambda}}. (42)$$

The second equation of (39) allows us to write

$$\begin{cases}
dx = v(\alpha)\cos(\alpha)dt = -\frac{1}{g}v^2(\alpha)d\alpha \\
dy = v(\alpha)\sin(\alpha)dt = -\frac{1}{g}v^2(\alpha)\tan(\alpha)d\alpha
\end{cases}$$
(43)

such that, after integration, we get the positions of the projectile

$$\begin{cases} x(\alpha) &= -\frac{1}{g} \int_{\alpha_0}^{\alpha} v^2(u) du + x_0 \\ y(\alpha) &= -\frac{1}{g} \int_{\alpha_0}^{\alpha} v^2(u) \tan(u) du + y_0 \end{cases}, \tag{44}$$

where (x_0, y_0) is the initial position of the object.

Here, we are interested in the range D of the mobile. It can be computed by first determining the angle α_s for which $y(\alpha_s) = 0$. This angle may be computed by solving the nonlinear equation $y(\alpha_s) = 0$ with the algorithm of Newton, which writes

$$\alpha^{k+1} = \alpha^k - \frac{y(\alpha^k)}{y'(\alpha^k)} = \alpha^k - \frac{\int_{\alpha_0}^{\alpha^k} v^2(u) \tan(u) du}{v^2(\alpha^k) \tan(\alpha^k)}.$$

The value used to initiate the recurrence relation is $\alpha_s = -\alpha_0$ and the integral in the above formula, is evaluated using the Fejer's quadrature rule of type I [3]. In the next section, three input parameters of this problem will be considered as stochastic and a sensitivity analysis will be performed.

4.2.2. Study of the stochastic problem.

We now consider the deflagration of an object and we assume that the trajectory of each fragment of the object may be described by a stochastic process. For that, three independent input parameteres are considered as Gaussian processes with independent increments. They are the initial velocity V_t^0 , the starting angle α_t^0 and the limit velocity V_t^{lim} . The index $t \in [0, T_f]$ of the stochastic processes represent the location of the fragment onto the initial object. We assume that two fragments close to each other will be indexed by parameters (s,t) such that |s-t| is small. The quantity of interest, i.e. the range $D = D_t$ of the projectile, can also be considered as a stochastic process which is a nonlinear function of the entry parameters. This case study focuses on the influence of $\Delta_s^t V^0$, $\Delta_s^t \alpha^0$, and $\Delta_s^t V^{\text{lim}}$ on the range difference $\Delta_s^t D = D_t - D_s$ of two fragments initially located at position s and t. We assume that the input processes are Gaussian processes having independent increments with the following means and variances (for $t \in [0, T_f] = [0, 1]$:

- $$\begin{split} \bullet \ & \mathbb{E}(V_t^0) = 300 \text{ and } Var(V_t^0) = 40t \ ; \\ \bullet \ & \mathbb{E}(\alpha_t^0) = \pi/4 \text{ and } Var(\alpha_t^0) = 0.03t \ ; \\ \bullet \ & \mathbb{E}(V_t^{\text{lim}}) = 800 \text{ and } Var(V_t^{\text{lim}}) = 4000t \ . \end{split}$$

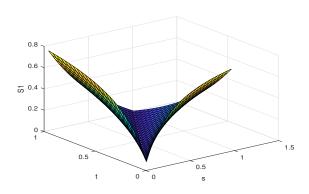


FIGURE 6. The first order Sobol'index S_1

The meta-model consists of a multivariate PC expansion of degree 12. Figures 6-11 show the first and second order Sobol' indices. According to the range of the values taken by S_{12} , S_{13} and S_{23} for all $(s,t) \in [0,1]^2$, we can say that the combined influence of two input stochastic processes onto $\Delta_s^t D$ can be neglected. For the first order indices S_2 and S_3 , (associated with $\Delta_s^t \alpha^0$ and $\Delta_s^t V^{\text{lim}}$, respectively), it is when $s \simeq 0$ (or $t \simeq 0$, by symmetry) that the influence associated with these indices is most important. On the other hand, S_1 (associated with $\Delta_s^t V^0$) shows a bigger influence of $\Delta_s^t V^0$ as $(s,t) \to (1,0) \text{ (or } (s,t) \to (0,1)).$

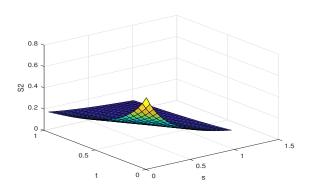


FIGURE 7. The first order Sobol'index S_2

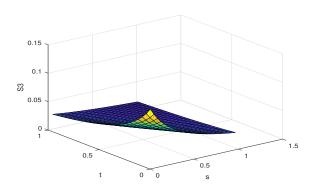


FIGURE 8. The first order Sobol'index S_3

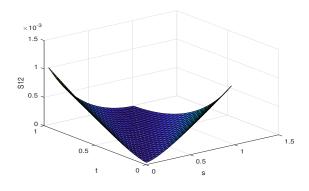


FIGURE 9. The second order Sobol'index $S_{1,2}$

5. Conclusion

In this paper, we have developed a numerical approach based on Sobol' indices to study the influence of input processes with independent increments that propagate into a physical system. In order to take into account the

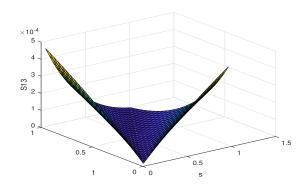


FIGURE 10. The second order Sobol'index S_{13}

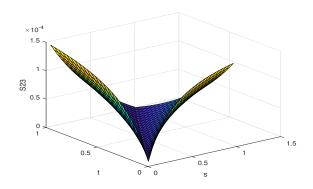


FIGURE 11. The second order Sobol'index $S_{2,3}$

specificity of stochastic processes, the study is carried out on the model output $Y_t - Y_s$ instead of Y_t . The fact that the input processes have independent increments allows us to reformulate the problem such that it can be treated as independent random variables. Therefore, polynomial chaos expansion may be used as meta-model and Sobol' indices can easily be computed from the PC coefficients. To illustrate the applicability of the proposed approach, one academic example based on Ishigami function is studied and a mechanical model without analytical solution is also treated. Further work should include the possibility to use other families of stochastic processes as input variables of our model.

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Appendix

In this appendix, we give the details of the expression appearing into the equations (36)-(37). Starting with the denominator of these equations, we have

$$V(Y_t - Y_s) = V(Y_t) + V(Y_s) - 2(\mathbb{E}(Y_t - Y_s) - \mathbb{E}(Y_t)\mathbb{E}(Y_s)),$$

$$= \mathbb{E}(Y_t^2) - (\mathbb{E}(Y_t))^2 + \mathbb{E}(Y_s^2) - (\mathbb{E}(Y_s))^2 - 2(\mathbb{E}(Y_tY_s) - \mathbb{E}(Y_t)\mathbb{E}(Y_s)),$$
with $\mathbb{E}(Y_t) = \frac{a}{2}(1 - e^{1 - e^{2t}})$, and
$$\mathbb{E}(Y_t^2) = \left(1 + 6b\left(\frac{t}{T(T - t)}\right)^2 + 105b^2\left(\frac{t}{T(T - t)}\right)^4\right)\frac{1 - e^{-2t}}{2}$$

$$+a^2\frac{3 - 4e^{1 - e^{2t}} + e^{4(1 - e^{2t})}}{8},$$

and eventually

$$\mathbb{E}(Y_t Y_s) = \left[1 + 3b \left(\frac{s}{T(T-s)}\right)^2 + 3b \left(\frac{t}{T(T-t)}\right)^2 + b^2 \left(\frac{s}{T(T-s)}\right)^2 \left(9 \left(\frac{t-s}{(T-t)(T-s)}\right)^2 + 90 \frac{t-s}{(T-t)(T-s)} \times \frac{s}{T(T-s)} + 105 \left(\frac{s}{T(T-s)}\right)^2\right)\right] e^{-\frac{1}{2}(t-s)} \frac{1-e^{-2s}}{2} + a^2 \left(\frac{1-e^{2s}-e^{2t}}{2} \times \frac{1-e^{4(1-e^{2s})}}{8} + \frac{1+e^{2s}-e^{2t}}{2} \times \frac{3-4e^{(1-e^{2s})}+e^{4(1-e^{2s})}}{8}\right).$$

For the numerator of the first order indices (see equations (36)), we have

$$V(\mathbb{E}(Y_t - Y_s | Z_t - Z_s)) = 0,$$

$$V(\mathbb{E}(Y_t - Y_s | B_t - B_s)) = e^{-s} \frac{1 - e^{-2(t-s)}}{2} \left(1 + 3b \left(\frac{t}{T(T-t)} \right)^2 \right)^2,$$

$$V(\mathbb{E}(Y_t - Y_s | M_t - M_s)) = \frac{a^2}{8} e^{2(1 - e^{2s})} \left(3 - 4e^{e^{2s} - e^{2t}} + e^{4(e^{2s} - e^{2t})} \right) - (\mathbb{E}(Y_t - Y_s))^2.$$

And finally, for the numerator of the second order indices (see equations (37)), we have

$$V(\mathbb{E}(Y_t - Y_s | B_t - B_s, M_t - M_s)) = 0,$$

$$V(\mathbb{E}(Y_t - Y_s | M_t - M_s, Z_t - Z_s)) = 0.$$

$$\begin{split} V(\mathbb{E}(Y_t - Y_s | B_t - B_s, Z_t - Z_s)) &= e^{-s} \left(\frac{1 - e^{-2(t - s)}}{2}\right) \left[1 + 105b^2 \left(\frac{t - s}{(T - t)(T - s)}\right)^4 \right. \\ &\quad + 9b^2 \left(\frac{s}{T(T - s)}\right)^4 \\ &\quad + 36b^2 \left(\frac{s}{T(T - s)}\right)^3 \left(\frac{t - s}{(T - t)(T - s)}\right) \\ &\quad + 126b^2 \left(\frac{s}{T(T - s)}\right)^2 \left(\frac{t - s}{(T - t)(T - s)}\right)^2 \\ &\quad + 180b^2 \left(\frac{s}{T(T - s)}\right) \left(\frac{t - s}{(T - t)(T - s)}\right)^3 \\ &\quad + 6b \left(\frac{s}{T(T - s)}\right)^2 + 6b \left(\frac{t - s}{(T - t)(T - s)}\right)^2 \\ &\quad + 12b \left(\frac{s}{T(T - s)}\right) \left(\frac{t - s}{(T - t)(T - s)}\right) \right]. \end{split}$$

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EMELINE GAYRARD, LABORATOIRE DE MATHÉMATIQUES BLAISE PASCAL (LMBP), CNRS UMR 6620, UNIVERSITÉ CLERMONT AUVERGNE, CAMPUS UNIVERSITAIRE DES CÉZEAUX, 3 PLACE VASARELY, TSA 60026 / CS 60026, 63 178 AUBIÈRE CEDEX FRANCE AND CEA / GRAMAT, BP 80200 46500 GRAMAT, FRANCE.

Email address: Emeline.Gayrard@uca.fr

CÉDRIC CHAUVIÈRE, LABORATOIRE DE MATHÉMATIQUES BLAISE PASCAL (LMBP), CNRS UMR 6620, UNIVERSITÉ CLERMONT AUVERGNE, CAMPUS UNIVERSITAIRE DES CÉZEAUX, 3 PLACE VASARELY, TSA 60026 / CS 60026, 63 178 AUBIÈRE CEDEX FRANCE.

Email address: Cedric.Chauviere@uca.fr

HACÈNE DJELLOUT, LABORATOIRE DE MATHÉMATIQUES BLAISE PASCAL (LMBP), CNRS UMR 6620, UNIVERSITÉ CLERMONT AUVERGNE, CAMPUS UNIVERSITAIRE DES CÉZEAUX, 3 PLACE VASARELY, TSA 60026 / CS 60026, 63 178 AUBIÈRE CEDEX FRANCE.

 $Email\ address: {\tt Hacene.Djellout@uca.fr}$

PIERRE BONNET, INSTITUT PASCAL, CNRS UMR 6602, UNIVERSITÉ CLERMONT AUVERGNE, CAMPUS UNIVERSITAIRE DES CÉZEAUX, 4 AVENUE BLAISE PASCAL, TSA 60026 / CS 60026, 63178 AUBIÈRE CEDEX, FRANCE.

 $Email\ address: {\tt pierre.bonnet@univ-bpclermont.fr}$

DON-PIERRE ZAPPA, CEA / GRAMAT, BP 80200 46500 GRAMAT, FRANCE. *Email address*: Don-Pierre.ZAPPA@CEA.FR